CompassCDS
Version 4.1.0
Release Notes

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What's New in CompassCDS 4.1.0

CompassCDS Core

Agilent ICF Support – Agilent's Instrument Control Framework (ICF) is now supported and allows to instantly install and use ICF/RC.Net control drivers with the Agilent ICF Driver.

Remote Sequence Manager – Unlike in previous versions the Remote Sequence Manager (External Sequence) is not crashing anymore when executing a sequence. Consequently, with current version the Remote Sequence can be used again in Client/Server environment.

Control Drivers

CompassCDS 4.1.0 supports Agilent's Instrument Control Framework (ICF) and related RC.Net control drivers for Agilent HPLC and GC.

RC.Net control driver for Agilent HPLC

Installer loads control drivers for Agilent HPLC series 1100, 1120 & 1220 Compact, 1200 & 1200 Infinity, 1260 Infinity I, II, and 1290 Infinity II, including fraction collectors and ELSD.

RC.Net control driver for Agilent GC

Installer loads control drivers for Agilent GC series 6890/6850, 7890 A/B, 7820, and 9000 Intuvo including related headspace autosamplers.

Add-ons

CompassCDS AnIML Converter and Viewer

AnIML Converter converts CompassCDS chromatograms into a human readable animl file that can be used for long-term archiving and reviewing of CompassCDS raw data, meta data and results without compromise with the AnIML Viewer component independently of CompassCDS, and also used for extraction and upload of results into LIMS or SAP/ERP.

Notes

Available Instrument Control Drivers

RC.Net Control Drivers

RC.Net control driver for Agilent HPLC

Current version LC Drivers A.02.18

Installer loads control drivers for Agilent HPLC series 1100, 1120 & 1220 Compact, 1200 & 1200 Infinity, 1260 Infinity I, II, and 1290 Infinity II, including fraction collectors (G1364 A/B/C/D, G5664 A, G7159 B, G7166 A), single or clustered. Also, the ELSD models 380/385 (G4260 A & G4261 A), 1260 (G4260 B) and 1290 (G7102 A & G4261 B) are supported.

RC.Net control driver for Agilent GC
Current version GC Drivers B.01.03

Installer loads control drivers for Agilent GC series 6890/6850, 7890 A/B, 7820, and 9000 Intuvo including related headspace autosamplers G4556A (7697A, 11 vials), G4557A (7697A, 111 vials) and G1888A.

Common control drivers

Control Driver for Scion 400 Series GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the model 456, 436, 450 and 436 GCs as well as a separate driver for the Varian/Bruker 430 GC.

Control Driver for Varian 3800 Series GC
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the model Varian 3800 GC.

Control Driver for Varian 3900 Series GC
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the model Varian 3900 GC.

Control Driver for Varian SHS-40
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the static SHS-40 headspace autosampler.

Control Driver for CTC CombiPal
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for CTC CombiPAL and xt.

Control Driver for Valco SSV
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Valco SSV.

Control Drivers for NI Devices
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the NI-9181 & NI-9184 chassis as well as drivers for the NI-9219 (Analog data acquisition), NI-9401 (TTL/IO) and NI-9481 (Contact closure relay) module that fit into these chassis.

Analog – Digital data acquisition - NI-9184 4 Slot Chassis fitted with NI-9219 ADC module and also required NI-9401 TTL/IO for inject start input. NI-9481 relay module can be added to this configuration if required. Analog data acquisition is restricted to a single time base with up to 4 channels (detectors) with the current driver.

Contact closure relay control – Either 4 slots NI-9184 or single slot NI-9181 chassis fitted with NI-9481 relay module.

TTL/IO Start in/Start out control - Either 4 slots NI-9184 or single slot NI-9181 chassis fitted with NI-9401 relay module.

Control Driver for Varian STAR 800 & 850 MIB
Current Version: 1.0.0.190

The control driver for the STAR 800 & 850 MIB interface supports analog data acquisition (4 channels), contact closure relay (4), serial (4-8 channels) and GPIB (max 2 IEEE cards) communication.

Control Driver for Agilent 5890 GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Agilent 4890 & 5890 Series GCs and associated autosamplers.

Control Driver for Agilent 6890/6850 GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Agilent 6890 & 6850 I/II Series GCs and associated autosamplers.

Control Driver for Agilent 7890 A/B GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Agilent 7890 A/B Series GCs and associated autosamplers.

Control Driver for Agilent 1260 HPLC
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads common control drivers for HP/Agilent 1100, 1200 and 1260 HPLC modules.

Manual Injector
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

Time Control
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

Generic Column Tracker
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

General

CompassCDS DCOM Tool – A tool for automatically setting all Windows DCOM and folder permissions for client server installations has been created and is included with every CompassCDS DVD. Tool does not replace manual security settings on the CompassCDS\Server and \data folder. For details see the installation guide.

Installation - Before installing CompassCDS, check that the 'File and Printer Sharing for Microsoft Networks' component is installed. This component is listed in the network connections properties. When Internet Explorer 7.0 or Edge is installed on the host computer, at the end of CompassCDS installation, the InstallShield wizard sometimes hangs up and pressing the Finish button does not close the wizard. The only solution is to use Windows task manager and to kill the Setup.exe applications.

It is strongly recommended that the computer be rebooted at the end of the installation.

If the Amyuni PDF driver is failing to install ('spooler error'), locate the file PDFprinter_install.exe in the CompassCDS\client folder and add the –p flag (PDFprinter_install-p.exe) before re-executing the installation. The -p option prevents the install utility from trying to stop and restart the spooler.

If the Amyuni PDF driver is not working then check Windows registry setting. Go to HKEY_CURRENT_CONFIG, then PDF Compatible Printer Driver, Permissions: make sure that "everyone" is set with full control is set. If not, add this to the security settings.

The Configuration Manager audit trail is not automatically archived when uninstalling the software. If you need to recover the audit trail, archive the current audit trail before uninstalling CompassCDS.

Screen Savers and Power Management - It is recommended that all screen savers be disabled. It is better to use the Windows energy saving feature for the monitor. It is recommended that all power management properties be disabled (Standby/Hibernates).

Backup - When backing up CompassCDS files, do not back up the \SERVER directory (including its subdirectories). Doing so will cause the loss of chromatogram files (*.DATA) that were acquired while the backup was being done. It is also recommended to avoid backing up recently acquired CompassCDS Data files (< 5 hours). Backups can only be done if CompassCDS and the Configuration Manager isn't in use and the nexusdb Windows service has been stopped.

Closing the application - Users are also advised not to let a cursor remain within a grid (sequence, identification table, integration table, reprocessing list) when exiting CompassCDS or closing files. If this occurs, the following error message 'Cannot focus a disabled or invisible window' may appear. This message has no consequences, and if it occurs while a sequence is running, the sequence should just be left to terminate before CompassCDS is closed.

Acquisition - If the administrator modifies the configuration of a system in the CompassCDS Configuration Manager (for example, renames a detector, adds or removes a detector, etc.), the methods created before the system configuration modifications will be invalid for acquisition (quick start or sequence). Users will have to create new methods. If the administrator creates, deletes or modifies the name of a system while a user is already connected to a group/project that owns this system, it will be necessary to log in to CompassCDS again to refresh the system list.

Calibration Curve - When working in concentration versus response mode, the format modification functions in the calibration curve table are inverted: when the Quantity variable format is changed, the Area/Height format is changed and when the Area/Height format is changed, the Quantity variable is changed.

Chromatogram - When a sequence or a reprocessing list is open, and the chromatogram data section is displayed and then the sequence (or reprocessing list) is clicked in the browser, the chromatogram trace will not be redisplayed when the chromatogram data section is reselected.

Workaround: click on the method section of the chromatogram and then select the data section to refresh the screen.

Event annotations are not correctly displayed on the chromatogram after extracting an archived data version (get archive option).

Workaround: click on the integration method sub-section to refresh the display.

A calibration curve is created by a user owning the archive calibration curve profile. This curve is cleared and a new point is added by a user that does not own the archive calibration curve profile. Then the user that owns the calibration curve profile reprocesses a chromatogram (F6) with the current curve and then with (F5), the results change because the last archive is used instead of the current one. The workaround is that the last user (archive calibration curve) must save the calibration curve before recalculating the results by (F5).

Suppose a standard chromatogram contains 3 identified and quantified peaks named A, B and C. The user has the 'Use M and D factors for curve building' profile. Peak C is processed as peak A ('Use References' option checked in the calibration table). When both conditions are used, peak C quantity will be Qeq*M/D instead of Qeq (with Qeq: quantity calculated according to the calibration curve equation).

Workaround: create the following variable:

QTY REC: peak user formula, real.

QTY REC = IF((NAME='X');QTY*DIVFACTOR/MULFACTOR;QTY), with X=C in this example.

When the user does not have the right to overwrite data and the data file name already exists, a date/time suffix is automatically added. This timestamp is always displayed with the English date/time format: Month2_Day2_Year4 whatever the regional settings of the PC are.

Electronic Signature - When you have validated your signature in the user identification for sign-off window, press the Close button to exit the window and not the 'X' button in the upper right corner of the window. For this operation, the Windows 'X' button is the same as the Cancel button. If the Windows 'X' button is used, the signature will not be applied. Suppose the user has the batch sign at once profile and a chromatogram has been excluded mistakenly from the list of files to be signed, it is then impossible to sign the corresponding chromatogram.

File Import - If a .CDF file is opened and reprocessed (F6 function) with an external method, no preview is available when selecting the resulting DATA file in the open file window and the absorbance values are null.

Workaround: after opening the .cdf file, save it before reprocessing it.

When importing an AIA file (.CDF) or a Star Workstation chromatogram (.RUN), save it before reintegrating it or reprocessing it.

Method - When printing the control method, a blank page is printed at the end. The control parameters are not printed if you open a chromatogram or a method and then change some method parameters (integration events for instance) before printing.

Workaround: save the method (or chromatogram) before printing.

Only methods created in the project in which the current user is logged are available in the sequence or quick start wizard. If a method created in project 1 is saved as another name in project 2, when logged in project 2 this new method will not be displayed in the sequence and quick start screens.

Method Templates - When creating a new method from template, some acquisition parameters are not imported from the template (run name, run ID, description, vial and rack numbers, injection volume, run length, dead time, specific channel option). Do not uncheck channels or injectors before saving a method as template.

Open File - In the chromatogram open file, only the first line of the run information is displayed in the information field.

PDF Export Plug-In - If the PDF Export plug-in needs to be used with the remote sequence feature, modify the external sequence engine service of the CompassCDS system to run as following:

From Windows, select Start/Control Panel/Administrative Tools/ Services

Locate the service named 'External Sequence engine – SYSTEM_1' (if the CompassCDS system to run is SYSTEM_1).

Right-click on this service and select 'Properties', then select the Log On tab.

Select the 'This account' option and select the account information (account name, password and password confirmation) for the account that will be used to start the service. Note that this account should have a default printer defined and a non-blank password.

In the main Services window, right-click on the service that was just modified and stop it so that the changes are taken into account next time the service is started.

Prep-Ahead - Suppose the prep vial number entered in the sequence is N. The real prep vial number taken into account will be N-1.

Using multi-injection per line is not possible in the sequence when working with prep-ahead.

Quick Start - It is not possible to add a summary report (with the add button) from the quick start screen. For multiple injector systems, the export is always performed at the end of the quick start, even though this option has been unchecked in the method properties.

Reprocessing List - If the chromatogram does not contain an acquisition method section (AIA files imported in CompassCDS, etc.), the method name used to reprocess this data will not be automatically imported in the reprocessing list. You must load it manually. The only way to stop a reprocessing list with the bracketing option checked is to close it. The stop button is not available during the calculation step. Do not use the fill block option while the processing list is running. More generally, use the pause option to make any changes when the reprocessing list is running. Assume several chromatograms (A, B, C and D) have been reprocessed with A as a blank and the other ones as standards. Then some of them were modified, the changes were saved, and they were imported into a reprocessing list after sorting them by the modification date in the file open window (for example: D, C, B and A). In the reprocessing list, the files will be displayed in the same order; D, C, B and A, but A will be identified as an unknown instead of a blank. After restoring the initial order (A, B, C and D), redefining the correct sample type for chromatogram A, and running the reprocessing list, it appears that the blank chromatogram subtracted for chromatograms B, C and D is not A.

Reprocessing Single - When manual operation (manual integration or manual identification) has been performed, do not change chromatogram properties (M, D, internal standard quantity, ….) directly from the reprocessing single screen. Firstly, change the required values from the chromatogram itself (by using the chromatogram properties button), then select the reprocessing single option and reprocess the chromatogram. Assume at least two chromatograms (A and B) are opened and are using the internal standard calibration mode. Chromatogram A is selected from the browser. In the reprocessing single window, after selecting chromatogram B and pressing the properties button, it is not possible to enter the internal standard value (the field is grayed out). The workaround is to close the reprocessing window and to select chromatogram B. Then it will be possible to edit the internal standard field directly from the reprocessing window.

Sequence - If a cell in the 'number of injections' column (displayed in second position after the 'Run#' column) is selected (without putting the cursor in it) and the value 0 is entered, CompassCDS will be frozen. You must end the task to restore CompassCDS operation. Do not use the copy and paste commands to duplicate the calibration cell content. If you select another file in the browser or open another file, an error will appear. The workaround is to use the fill block feature.

On a system with two injectors, if you uncheck one of the injectors and restart the sequence by overwriting the data files, a second injection date (corresponding to the acquisition date of the active

injector) will appear in the run log screen (available in the acquisition sub-section of the chromatogram method). This second date is only displayed for the files that are associated with the injector that is not active.

For multiple-injector systems, select the required sub-system to create fill blocks. When multiple injections are defined per line, if you want to make fill blocks or disable a line:

First, define 1 as number of injections and make the required changes, then enter the desired number of injections.

Otherwise the changes will only be applied on the first injection of the given run.

When several injections are defined per line, do not use the arrows to validate the entries in the No of injections column. It may induce a double numbering of the line index column when printing the sequence.

The processing parameters (pre-processing, integration, identification, calibration…) are disabled in the method properties and are also applied at the end of the acquisition. This is a normal behavior to ensure coherence between the chromatogram method and the results.

When renaming an existing project from the Configuration Manager, the old methods are no longer available from a sequence created before the project is renamed. The workaround is to create a new sequence.

Sequence blank runs - When a sequence that usually starts with line in which the Sample type is defined as a Blank, what happens, is that for all the subsequent runs the blank run is automatically subtracted from each chromatogram. The resulting data-files will all have a line in the pre-processing section, pointing to the blank run. When processed or re-processed the resulting reports show all variables (such as method name, or start run time, username, etc.) as 'not defined' and the peak names are missing from these chromatograms and the results table will be empty. When manually re-processed, these files return a message saying 'processing: aborted'. Only re-processing with the original Global method file resolves this issue, because the line pointing to the sequence blank will be removed.

Workaround: Do not select Sample type Blank if the intention is to first run a blank sample to ensure no sample carry over. Select Sample type Unknown instead.

Star Workstation .RUN file import – Users can once again import legacy Star Workstation .RUN files. CompassCDS will automatically import a copy of the .RUN file and convert it into a .DATA file. Peak names will also be imported.

Summary Report - An extra-printing may occur during the sequence in the following conditions:

The 'print after a new warning' option has been configured.

A warning in the sequence generates the printing of the summary report.

This extra-printing will be performed at the end of each following acquisition only if the chromatogram corresponds to a sample type that is not automatically added into the summary report.

Do not reprocess the same chromatogram several times within a reprocessing list with the same method including the same summary report.

It is highly recommended that the summary report name be defined directly in the method (summary report sub-section) rather than defining its name directly from the method properties screen in the sequence (or reprocessing list).

Suitability Tests - The sample type is taken into account for the suitability actions only that means a result is computed for each suitability test whatever the sample type is. This is a normal behavior.

Temporary Files - The *.DEC files can be deleted manually. One DEC file is created per sequence. The deletion has no impact on the normal use of the software. These files are normally stored in C:\WINNT or C:\TEMP. Use the Start/Find option to be sure to find all the *.DEC files.

Variables - The Deltat variable (1/acquisition rate) is displayed with 2 decimals in the chromatogram properties. Depending on the acquisition rate, 0.00 may be displayed. The workaround is to create a new global user formula variable (formula: = DELTAT) and to select more decimals to display.

The value of the Samplename variable is always N.A. A workaround is to use the Runname variable that corresponds to the chromatogram's name instead of this one.

It is not recommended to change the type of a user formula variable as results are not automatically updated after a reprocess (F6). The workaround is to reintegrate (F5) the chromatogram before reprocessing of the chromatogram.

Notes on CompassCDS Report Editor

Open File - Use the Open button to open a report style. Double-clicking on the file name may cause some coordinates to be changed.

Chromatogram - The default format for peak and group reports corresponds to the format defined in the chromatogram whereas the chromatogram default format corresponds to the software format.

Printing the Method - Peak user-input variables applied to data are not saved within the method, and therefore are not printed in the Chromatogram Method Report. The reference column is always printed as part of the peak identification table in the Chromatogram Method Report. If no reference peak is defined, the column will be printed with the header: 'Ref?', but left blank.

Text and Label - If defining $PAGENUM or $PAGECOUNT variables in a text or label object and that the variable name is cut in the report template (because the text /label object is not large enough), then the value of the variable is not printed in the report but $PAGENUM or $PAGECOUNT is printed. Enlarge the text or label object in the report template to solve the issue.

Notes on CompassCDS Configuration Manager

General - When the NexusDB Server service has been stopped for any reason, it should be manually restarted otherwise it will not be possible to log in the Configuration Manager.

The following limitations are present in the Configuration Manager compared to versions prior to 1.8:

Group, project, user, user profile, administrator profile, system and station names do not exceed 40 characters.

User initials do not exceed 4 characters.

Accents, parentheses, ‘, “, ^, ¨, or µ characters are forbidden in item names (group, project, user, profile, system and station). Parentheses are also forbidden in injector and detector names.

These limitations have been added to fix or prevent potential problems.

Configuration - After changing some parameters from the Configuration menu (security, electronic signature…. Parameters), it is recommended to exit CompassCDS and to login again instead of selecting the Session/New Login option.

By default, a Group1 is created, a default template path is defined in its properties: C:\CompassCDS\data\template, but the corresponding directory does not exist on the station. The workaround is to edit the group1 properties, and answer yes to the message prompting the user to create the template path.

Printing System Configuration - When you print the system configuration, an additional blank page is printed.

System - When renaming some channels, detectors are not sorted by alphabetical order in the system tree view. Moreover, when creating a system with several injectors and detectors, they are not sorted by alphabetical order before the database is refreshed (F5). When some drivers have been updated, the corresponding devices version may not be refreshed properly in the system properties. The workaround is to refresh the view (F5).

System Properties - When you change the system name or the signal unit in the configuration manager, you need to restart the CompassCDS session to update the acquisition window. Otherwise, the old name and unit will be displayed.

Users - Defining the same user several times with different profiles in a given group/project is not possible.

Plug-ins and Add-ons

Enhanced Chromatogram Report – New version replaces the Multi-Channel Chromatogram Report. Users can create customized reports as a single report for up to 4 channels, and peak and group results can be displayed separated by channel or combined into one single table each. Supports now also QTY normalization over up to 4 channels. Report can be executed in direct mode via the toolbar menu or during reprocessing of the chromatogram.

1-Button Interface - An easy-to-install simplified graphical user interface with a CompassCDS administrator accessible configuration screen that enables runs to be set up by operators using individual icons to specify the type and number of sample runs, multi-level calibrations, control sample and blank runs and, if required, continuous looping runs for routine samples taken from the continuous gas or liquid flow or storage tanks via valve injection. The new version also supports sample injection from controlled autosamplers, and entering of text that is displayed thereafter in the run info field of the chromatogram.

Currently the 1-Button interface can only be used with one CompassCDS Project per logon even though the All Projects mode can be selected.

Hydrocarbon Reporting Tool – Special plugin for the hydrocarbon processing industry focusing on ASTM, GPA and ISO based calculations for gases and liquids. Report and calculations can be flexibly setup and executed in direct mode or as a post-run process. Calculations include component, summary and extended calculations. Additionally, the Hydrocarbon Calculation Tool supports custom calculations and automated export of report details and calculated results in XML format.

CompassCDS AnIML Converter - Add-on for long-term archiving of chromatogram raw data, meta data and results in a human readable AnIML file format. AnIML file can be also used to extract and upload of chromatogram results into LIMS or SAP/ERP. Converter can be used in automatic mode as post-run executable file, or by drag & drop of chromatograms into the CompassCDS Viewer component.

CompassCDS AnIML Viewer – Viewer component for AnIML files. Allows to display and fully review and process chromatogram details (raw data, meta data and results) without compromise even after a long period of time and the need to have CompassCDS available on the computer.